**Supporting Information**

**Table S1.** Designing of library of pyranooxazoles

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Parent Compound | C. No. | R1 | R2 | R3 | C. No. | R1 | R2 | R3 |
| 1 | -NH2 | -Br | -Br | 12 | -OH | -OCH3 | -Cl |
| 2 | -OCH3 | -Br | -Br | 13 | -OH | -NO2 | -OCH3 |
| 3 | -OH | -Br | -Br | 14 | -OH | -CH3 | -I |
| 4 | -OH | -Br | -Cl | 15 | -OH | -CH3 | -Cl |
| 5 | -OH | -Br | -NO2 | 16 | -OH | -Cl | -F |
| 6 | -OCH3 | -OCH3 | -Br | 17 | -OH | -CH3 | -F |
| 7 | -OH | -NO2 | -Br | 18 | -F | -F | -F |
| 8 | -OH | -OCH3 | -Br | 19 | -OH | -F | -F |
| 9 | -OH | -Cl | -Cl | 20 | -OH | -F | -Br |
| 10 | -Cl | -Cl | -Cl | 21 | -F | -Cl | -CF3 |
| 11 | -OCH3 | -OCH3 | -Cl |  |  |  |  |
| Parent Compound | C. No. | R1 | R3 | R4 | C. No. | R1 | R3 | R4 |
| 22 | -I | -CH3 | -CH3 | 28 | -Br | -OCH3 | -OH |
| 23 | -I | -OH | -CH3 | 29 | -Br | -OCH3 | -OCH3 |
| 24 | -Br | -F | -Br | 30 | -OCH3 | -OCH3 | -Br |
| 25 | -F | -OCH3 | -CH3 |  |  |  |  |
| 26 | -F | -F | -F |  |  |  |  |
| 27 | -F | -F | -OCH3 |  |  |  |  |
| Parent Compound | C. No. | R1 | R4 | R5 | C. No. | R1 | R4 | R5 |
| 31 | -NO2 | -OCH3 | -OCH3 | 36 | -Cl | -Cl | -Cl |
| 32 | -F | -Cl | -F | 37 | -Br | -CH3 | -OH |
| 33 | -Cl | -OCH3 | -F |  |  |  |  |
| 34 | -Cl | -CH3 | -F |  |  |  |  |
| 35 | -F | -F | -Cl |  |  |  |  |
| Parent Compound | C. No. | R1 | R3 | R5 |  |  |  |  |
| 38 | -F | -OCH3 | -F |  |  |  |  |
| 39 | -F | -Cl | -F |  |  |  |  |
| 40 | -F | -CN | -F |  |  |  |  |
| 41 | -F | -Br | -F |  |  |  |  |
|  |  |  |  |  |  |  |  |
| Parent Compound | C. No. | R2 | R­3 | R4 | C. No. | R2 | R3 | R4 |
| 42 | -Br | -OH | -Br | 48 | -Cl | -OH | -F |
| 43 | -Br | -OCH3 | -OCH3 | 49 | -Cl | -OH | -OCH3 |
| 44 | -OCH3 | -OH | -I | 50 | -Cl | -OCH3 | -OCH3 |
| 45 | -OCH3 | -OCH3 | -I | 51 | -Br | -OH | -OCH3 |
| 46 | -F | -F | -F | 52 | -Br | -OH | -Cl |
| 47 | -F | -OH | -OCH3 |  |  |  |  |
|  |  |  |  |  |  |  |  |
| Parent Compound | C. No. | R2 | R3 |  | C. No. | R2 | R3 |  |
| 53 | -OCH3 | -OCH2CH2Br |  | 67 | -F | -Br |  |
| 54 | -Br | -CH3 |  | 68 | -OCH3 | -F |  |
| 55 | -NO2 | -Br |  | 69 | -NO2 | -F |  |
| 56 | -Br | -OCH3 |  | 70 | -Cl | -F |  |
| 57 | -Br | -OH |  | 71 | -CH3 | -F |  |
| 58 | -OH | -Cl |  | 72 | -CN | -F |  |
| 59 | -NO2 | -Cl |  | 73 | -Br | -F |  |
| 60 | -Cl | -CH3 |  | 74 | -OH | -OCF2H |  |
| 61 | -OCH3 | I |  | 75 | -CF3 | -F |  |
| 62 | -OCH3 | -F |  | 76 | -CF3 | -Cl |  |
| 63 | -F | -F |  | 77 | -CF3 | -CF3 |  |
| 64 | -F | -Cl |  | 78 | -Cl | -OH |  |
| 65 | -F | -CH3 |  | 79 | -Cl | -OCH3 |  |
| 66 | -F | -CN |  | 80 | -Cl | -Cl |  |
| Parent Compound | C. No. | R1 | R4 |  | C. No. | R1 | R4 |  |
| 81 | -Br | -Br |  | 93 | -F | -NO2 |  |
| 82 | -Br | -OCH3 |  | 94 | -F | -F |  |
| 83 | -Br | -OH |  | 95 | -F | -Cl |  |
| 84 | -OCH3 | -Br |  | 96 | -F | -Br |  |
| 85 | -OH | -Br |  | 97 | -F | -CF3 |  |
| 86 | -NO2 | -OH |  | 98 | -Cl | -CF3 |  |
| 87 | -I | -OCH3 |  | 99 | -CF3 | -CF3 |  |
| 88 | -OH | -F |  | 100 | -OH | -Cl |  |
| 89 | -OCH3 | -F |  | 101 | -NO2 | -Cl |  |
| 90 | -CH3 | -F |  | 102 | -Cl | -NO2 |  |
| 91 | -Br | -F |  | 103 | -Cl | -Cl |  |
| 92 | -F | -OCH3 |  |  |  |  |  |
| Parent Compound | C. No. | R1 | R3 |  | C. No. | R1 | R3 |  |
| 104 | -NO2 | -NO2 |  | 115 | -Cl | -OH |  |
| 105 | -Cl | -F |  | 116 | -Cl | -Cl |  |
| 106 | -CH3 | -F |  | 117 | -Cl | -CH3 |  |
| 107 | -F | -OCH3 |  | 118 | -OH | -Br |  |
| 108 | -F | -F |  | 119 | -OCH3 | -Br |  |
| 109 | -F | -Br |  | 120 | -NO2 | -Br |  |
| 110 | -NO2 | -CF3 |  | 121 | -Br | -OCH3 |  |
| 111 | -F | -CF3 |  | 122 | -Br | -Cl |  |
| 112 | -CF3 | -F |  | 123 | -Br | -CH3 |  |
| 113 | -OCH3 | -Cl |  |  |  |  |  |
| 114 | -NO2 | -Cl |  |  |  |  |  |
| Parent Compound | C. No. | R2 | R4 |  | C. No. | R2 | R4 |  |
| 124 | -OH | -NO2 |  | 129 | -Br | -NO2 |  |
| 125 | -F | -F |  | 130 | -Br | -Cl |  |
| 126 | -CF3 | -F |  | 131 | -Br | -Br |  |
| 127 | -CF3 | -CF3 |  |  |  |  |  |
| 128 | -Cl | -Cl |  |  |  |  |  |
|  |  |  |  |  |  |  |  |
| Parent Compound | C. No. | R2 | R5 |  | C. No. | R2 | R5 |  |
| 132 | -CN | -OCH3 |  | 137 | -NO2 | -Cl |  |
| 133 | -I | -OH |  | 138 | -Cl | -Cl |  |
| 134 | -I | -OCH3 |  | 139 | -CH3 | -Cl |  |
| 135 | -F | -I |  |  |  |  |  |
| 136 | -OH | -Cl |  |  |  |  |  |
|  |  |  |  |  |  |  |  |
| Parent Compound | C. No. | R1 | R2 |  | C. No. | R1 | R2 |  |
| 140 | -OH | -NO2 |  | 146 | -F | -CF3 |  |
| 141 | -F | -OCH3 |  | 147 | -Cl | -CF3 |  |
| 142 | -F | -F |  | 148 | -OH | -OH |  |
| 143 | -F | -Cl |  | 149 | -OH | -OCH3 |  |
| 144 | -OH | -F |  | 150 | -OH | -Br |  |
| 145 | -CH3 | -F |  | 151 | -Br | -OH |  |
| Parent Compound | C. No. | R1 | R5 |  | C. No. | R1 | R5-Cl-CH3-F-CF3 |
| 152 | -NO2 | -NO2 |  | 156 | -F |
| 153 | -I | -F |  | 157 | -F |
| 154 | -F | -OCH3 |  | 158 | -Br |
| 155 | -F | -F |  | 159 | -F |
| Parent Compound | C. No. | R1 | C. No. | R1 | Parent Compound | C. No | R3 | C. No. | R3 |
| 160 | -CN | 164 | -Cl | 168 | -CN | 173 | -SCF3 |
| 161 | -I | 165 | -Br | 169 | -I | 174 | -OCF3 |
| 162 | -F | 166 | -H | 170 | -F | 175 | -CF3 |
| 163 | -CF3 | 167 | -NO2 | 171 | -OCF2H | 176 | -Cl |
|  |  |  |  | 172 | -OCF2CF2H | 177 | -Br |
|  |  |  |  |  |  |  |  |
| Parent Compound | C. No. | R2 | C. No. | R2 |  |  |  |  |
| 178 | -NO2 | 184 | -OCF2CF2H |  |  |  |  |
| 179 | -CN | 185 | -OCF3 |  |  |  |  |
| 180 | -I | 186 | -CF3 |  |  |  |  |
| 181 | -F | 187 | -Cl |  |  |  |  |
| 182 | -OCF2H | 188 | -NH2 |  |  |  |  |
| 183 | -CF2H | 189 | -Br |  |  |  |  |
|  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |
| Parent Compound | C. No. | R1 | R2 | R3 |  |  |  |  |
| 190 | -I | -OH | -OCH3 |  |  |  |  |
| 191 | -F | -F | -F |  |  |  |  |
| 192 | -Cl | -OH | -OCH3 |  |  |  |  |
| 193 | -Cl | -OCH3 | -CH3 |  |  |  |  |
| 194 | -Br | -OH | -OCH3 |  |  |  |  |
|  |  |  |  |  |  |  |  |
| Parent Compound | C. No. | R1 | R2 | R3 | R4 |  |  |  |
| 195 | -OH | -Br | -OCH3 | -Br |  |  |  |
| 196 | -Br | -OCH3 | -OCH3 | -OCH3 |  |  |  |
|  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |
| Parent Compound | C. No. | R1 | R2 | R4 | R5 |  |  |  |
| 197 | -F | -F | -F | -F |  |  |  |
| 198 | -Br | -Br | -OCH3 | -OH |  |  |  |
|  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |

**Table S2.** Total binding energy of pyranooxazoles (200 molecules) using iGemDock as mentioned in Table 1.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| C. No. | T. Energy(kcal/mol) | C. No.  | T. Energy (kcal/mol) | C. No. | T. Energy (kcal/mol) | C. No. | T. Energy (kcal/mol) | C. No. | T. Energy (kcal/mol) |
| **104** | **-151.024** | 140 | -110.173 | 64 | -102.57 | 51 | -87.2158 | 79 | -77.4713 |
| **152** | **-130.99** | 25 | -109.699 | 155 | -102.409 | 111 | -87.1946 | 37 | -77.4342 |
| **174** | **-128.705** | 89 | -109.629 | 200 | -102.226 | 194 | -86.6292 | 148 | -77.114 |
| **168** | **-124.486** | 17 | -109.585 | 157 | -102.044 | 8 | -86.5221 | 100 | -76.4632 |
| **171** | **-122.982** | 162 | -109.475 | 32 | -101.317 | 49 | -85.6815 | 52 | -75.9773 |
| 62 | -122.981 | 24 | -109.406 | 61 | -101.206 | 6 | -85.2163 | 151 | -75.6573 |
| 23 | -122.917 | 65 | -108.676 | 143 | -100.802 | 11 | -84.8024 | 83 | -75.1011 |
| 145 | -122.906 | 134 | -108.547 | 154 | -100.761 | 113 | -84.6691 | 42 | -74.9199 |
| 13 | -122.389 | 144 | -108.456 | 91 | -100.694 | 185 | -84.6178 | 123 | -74.7213 |
| 199 | -121.143 | 153 | -108.211 | 105 | -100.235 | 147 | -84.4099 | 85 | -74.3806 |
| 31 | -121.047 | 38 | -108.149 | 106 | -100.178 | 195 | -83.2766 | 122 | -74.1907 |
| 48 | -120.777 | 87 | -108.097 | 161 | -99.7019 | 21 | -83.1945 | 1 | -74.1734 |
| 93 | -120.455 | 169 | -108.037 | 71 | -99.3197 | 112 | -83.0898 | 10 | -74.0032 |
| 124 | -120.449 | 109 | -108.026 | 19 | -99.0802 | 127 | -83.0275 | 4 | -73.8214 |
| 26 | -119.379 | 45 | -107.668 | 158 | -99.0542 | 28 | -82.9719 | 136 | -73.6993 |
| 178 | -119.375 | 86 | -107.375 | 156 | -98.8142 | 76 | -82.9572 | 56 | -73.6737 |
| 172 | -118.848 | 18 | -107.286 | 70 | -98.5523 | 30 | -82.5174 | 117 | -73.4756 |
| 74 | -118.154 | 182 | -106.832 | 120 | -98.5323 | 119 | -82.4378 | 36 | -73.458 |
| 69 | -117.871 | 27 | -106.639 | 5 | -98.0773 | 43 | -82.2282 | 82 | -73.4276 |
| 47 | -117.835 | 133 | -106.631 | 110 | -97.3193 | 175 | -81.6704 | 118 | -73.0507 |
| 41 | -117.407 | 135 | -106.355 | 114 | -97.1842 | 84 | -81.2327 | 121 | -73.0467 |
| 141 | -116.975 | 183 | -106.16 | 99 | -97.0871 | 150 | -81.1575 | 116 | -72.6679 |
| 66 | -116.365 | 22 | -105.598 | 96 | -96.8865 | 12 | -81.117 | 103 | -71.8936 |
| 132 | -116.238 | 197 | -105.386 | 7 | -96.8393 | 192 | -81.0154 | 58 | -71.421 |
| 108 | -115.676 | 170 | -105.152 | 180 | -95.8013 | 2 | -80.7301 | 81 | -71.3117 |
| 184 | -114.869 | 33 | -105.056 | 76 | -95.5367 | 149 | -80.6729 | 130 | -70.3479 |
| 125 | -114.502 | 15 | -104.998 | 53 | -93.9088 | 9 | -80.6572 | 128 | -70.2807 |
| 46 | -114.222 | 181 | -104.976 | 167 | -93.6226 | 159 | -80.5987 | 60 | -69.9664 |
| 16 | -114.092 | 68 | -104.784 | 5 | -92.7678 | 50 | -80.5971 | 54 | -69.756 |
| 179 | -113.572 | 20 | -104.415 | 129 | -92.0723 | 97 | -79.9969 | 131 | -69.0474 |
| 191 | -113.184 | 39 | -104.23 | 188 | -91.4483 | 186 | -79.6266 | 80 | -68.9514 |
| 95 | -112.086 | 14 | -104.221 | 198 | -91.3247 | 115 | -79.5783 | 165 | -68.8333 |
| 44 | -111.829 | 35 | -104.191 | 196 | -91.2419 | 193 | -79.2492 | 138 | -68.5833 |
| 107 | -111.6 | 92 | -104.03 | 55 | -90.8119 | 78 | -78.6577 | 139 | -67.9901 |
| 72 | -111.531 | 90 | -104.024 | 59 | -89.8334 | 57 | -78.6351 | 164 | -67.7933 |
| 40 | -111.406 | 88 | -103.967 | 137 | -89.0885 | 146 | -78.4184 | 187 | -67.3049 |
| 160 | -111.283 | 173 | -103.844 | 102 | -88.7829 | 75 | -78.1454 | 177 | -67.2161 |
| 67 | -110.527 | 94 | -103.821 | 29 | -88.2532 | 98 | -77.9431 | 176 | -66.1245 |
| 63 | -110.369 | 190 | -103.079 | 126 | -88.0658 | 3 | -77.65 | 189 | -65.3745 |
| 34 | -110.365 | 73 | -102.727 | 101 | -87.6749 | 163 | -77.6302 | 166 | -62.3661 |